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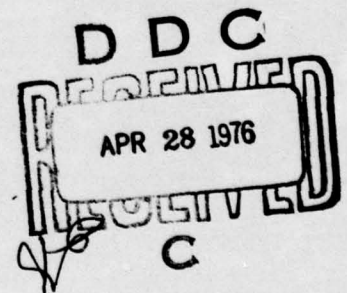
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Calculation of Effective Ozone Absorption Coefficients for a Rocketborne Ozonesonde

by
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MARCH 1977

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FOREWORD

This report describes the measurement of the transmittance of filters used in a rocketborne ozonesonde and the calculation of effective ozone absorption coefficients from the transmittance data.

The purpose of the report is to document the measurement procedures and calculations and to give explicit instructions for running the computer programs.

The study was supported by NASA.

This report was reviewed for technical accuracy by A. Krueger of NASA.

Released by
E. B. ROYCE, Head
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31 March 1977

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I. INTRODUCTION

Ozone has intense absorption in the middle ultraviolet region and serves to shield the earth from the sun's radiation in this region. A knowledge of the spacial and temporal distribution of ozone is important in the study of the chemistry of the atmosphere and in the evaluation of the impact of man-made catalytic trace constituents upon the ozone shield.

The attenuation of solar energy by ozone may be used to determine the height distribution of ozone in the upper atmosphere. The optical measurements needed to determine the attenuation are made by a sequential-sampling ultraviolet filter photometer which is carried aloft by a rocket and which descends on a parachute. The design of the ozonesonde has been described;¹ the system being used currently is a modification* of that described in the reference. The ozone concentration measurements are made at altitudes of 20 to 70 km.

This report describes the measurement of the transmittance of filters used in the rocketborne ozonesonde and the treatment of the data by computer to calculate effective ozone absorption coefficients. The application and operation of the programs are described. The report is intended for those interested in the measurement procedures and calculations used in obtaining effective ozone coefficients. Program listings are not given but may be obtained upon request.

II. EFFECTIVE OZONE ABSORPTION COEFFICIENT

The maximum ozone absorption occurs at 2553 \AA , and measurable absorption is found to approximately 3300 \AA . If the attenuation of direct sunlight by the earth's atmosphere is assumed to be due solely to absorption by ozone and to Rayleigh scattering, then the intensity of direct sunlight is given by the expression (Beer's law)

* The modified system will be described in a NASA report by Krueger *et al.*

¹ Naval Weapons Center. *Rocket Ozonesonde (ROCOZ) - Design and Development*, by A. J. Krueger and W. R. McBride. China Lake, Calif., NWC, July 1968. 40 pp. (NWC TP 4512, publication UNCLASSIFIED.)

$$I(\lambda, h) = I_o(\lambda) e^{-\alpha(\lambda) \cdot x(h)} e^{-\beta(\lambda) m(h)}, \quad (1)$$

where $I(\lambda, h)$ is the intensity at wavelength λ and height h (the other quantities are defined below). Since the filters have finite optical bandwidths, the monochromatic absorption coefficients $\alpha(\lambda)$ are replaced by an effective absorption coefficient which is defined as the weighted mean value of the ozone absorption coefficients.

$$\alpha_j(x, m) = -\frac{1}{x} \ln \frac{\int I_o(\lambda) Q(\lambda) S(\lambda) F_j(\lambda) e^{-\alpha(\lambda) \cdot x} e^{-\beta(\lambda) m} d\lambda}{\int I_o(\lambda) Q(\lambda) S(\lambda) F_j(\lambda) e^{-\beta(\lambda) m} d\lambda}, \quad (2)$$

where

$\alpha_j(x, m)$ = effective ozone absorption coefficient for the j^{th} filter

j = filter number

x = slant path ozone amount from height h above the earth to the top of the atmosphere

m = slant path air mass above height h

λ = wavelength

$I_o(\lambda)$ = extraterrestrial solar irradiance

$F_j(\lambda)$ = transmittance function for the j^{th} filter

$Q(\lambda)$ = photodetector response

$S(\lambda)$ = transmittance function for the diffuser plate

$\alpha(\lambda)$ = ozone absorption coefficient

$\beta(\lambda)$ = Rayleigh scattering coefficient.

This expression is evaluated numerically at 1-Å intervals.

The values employed for the extraterrestrial solar irradiance, the ozone absorption coefficients, the Rayleigh scattering coefficients, and the photodetector response were supplied by A. J. Krueger* of NASA, Goddard Space Flight Center, Greenbelt, Maryland. The transmittance function of the diffuser $S(\lambda)$ and the transmittance function of the filters $F(\lambda)$ come from laboratory measurements of all the filters and a few of the diffusers as described in the next section.

III. TRANSMITTANCE MEASUREMENTS

The transmittance of each filter and some of the diffusers is measured with a dual range (0 to 100%, 0 to 10%) Cary Model 14R spectrophotometer equipped with two encoders which convert shaft positions to digital form. Both analog and digital records of the data are made.

The pen position encoder (transmittance) is coupled to the pen drive mechanism; the encoder goes from -50 to +1050 counts for 360° of shaft rotation. A span of 1000 counts corresponds to a range of 0 to 100% transmittance (T) or 0 to 10%T depending upon the position of the range selection switch of the spectrophotometer. Thus, a change of one count corresponds to a change of 0.1%T on the 0 to 100%T range and to 0.01%T on the 0 to 10%T range. The zero of the pen (and hence, of the analog record) seldom corresponds to the zero of the encoder. For example, the encoder may give 28 counts when the pen is at its zero position. Then, on the 0 to 100%T range, an encoder reading of 1028 counts corresponds to 100%T. This offset between the zeroes of the pen and the encoder must be corrected for; the procedure and program for doing this are described later in this report. The wavelength mechanism of the

*The data supplied were arrived at in the following manner. The solar irradiance values were obtained by averaging a high resolution spectrum (Furukawa *et al.*²) over 1-Å intervals. The photodetector response was taken as a constant and set equal to one. The ozone absorption coefficients were taken from Vigroux³ and Inn and Tanaka.⁴ The Rayleigh scattering coefficients were calculated.¹

²National Center for Atmospheric Research. *Composite, High Resolution Solar Spectrum from 2080 to 3600 Å*, by P. M. Furukawa, P. L. Haagenson, and M. J. Scharberg. Boulder, Colo., NCAR, February 1967. (NCAR Technical Note No. 26, publication UNCLASSIFIED.)

³E. Vigroux. "Contribution à l'étude expérimentale de l'absorption de l'ozone," *Ann. Phys.*, Vol. 8 (1953), pp. 709-62.

⁴Edward C. Y. Inn and Yoshio Tanaka. "Ozone Absorption Coefficients in the Visible and Ultraviolet Regions," in *Ozone Chemistry and Technology*. Washington, D.C., American Chemical Society, 1959. *Advances in Chemistry Series #21*, pp. 263-68.

spectrophotometer is connected directly to an encoder which converts shaft position to digital form. One count on the encoder corresponds to 1 Å. The output of the encoders goes to a Datex SDS-1 spectrophotometer data recording system having a punched paper tape output. The control module of the SDS-1 system provides for the command to read out data and for the recording on tape of identification information in the form of a 10-digit number, each digit of which is manually set on one of 10 thumbwheel parameter switches. The system uses the IBM odd parity code given in Table 1 of Appendix A.

The 10-digit identification number is recorded twice at the beginning of every spectrum recorded on tape. The first six digits give the date the spectrum was recorded (month, day, year), the next two digits designate the filter assembly, and the last two digits give the spectrum number. Thus the identification number 1024751206 identifies the record which follows as being the 6th spectrum run on 24 October 1975 and shows that it is for filter assembly number 12. Next the transmittance (in digital counts) and wavelength data are recorded every angstrom. Tables showing the identification number record format and the transmittance-wavelength data record format are given in Appendix A.

A. TRANSMITTANCE OF FILTERS*

Narrow-band optical filters having bandpasses centered at approximately 2630, 2880, 3010, and 3200 Å and having half-widths of about 32 to 41 Å except for the 2630 Å narrow-band filter which has a half-width of about 103 to 109 Å, are used in conjunction with a broad-band filter to isolate narrow regions of the spectrum. The broad-band filter is made of single crystalline nickel sulfate hexahydrate sandwiched between plates of Corning 9863 glass and is used to isolate the ultraviolet region and block the visible region. The narrow-band filters are mounted in a rotatable filter wheel. The filter wheel and broad-band filter are mounted in the sample compartment of the spectrophotometer in such a manner that the monochromatic radiation passes through the narrow-band filter (mirror side towards incoming radiation), a 3/8-inch stop, and then the broad-band absorption filter. The spectra are scanned at 2.5 Å/sec from 3425 to 2500 Å. A short slit height is used to reduce the chance of inadvertent beam clipping by the filter wheel.

* The term filter without a modifier specifying narrow or broad will refer to a filter composed of two parts, one a narrow-band filter and one a broad-band filter. Thus, the term 3200-Å filter refers to the combination of a 3200 Å narrow-band filter with a broad-band filter.

The long wavelength tail of the 2630-Å filter has a small light leak which lies at a wavelength at which the atmosphere is far more transparent than it is at 2630 Å. Hence, the leak is important in the calculation of ozone concentrations. In order to examine the long wavelength tail of the 2650-Å filter on an extended range a neutral density screen of about 1%T is used to attenuate the reference beam of the spectrophotometer; this results in full scale on the 0 to 10% range of the instrument being approximately 0.1%T.

The transmittance of most of the filters was measured on the 0 to 10%T range except for a few whose transmittance exceeded 10%. Because the 100%T line of the instrument could not be made completely flat (i.e., independent of wavelength) with the available multipot adjustments of the spectrophotometer, the 100% line was recorded and used to correct filter spectra for small deviations of the 100% line from the value 100.

B. TRANSMITTANCE OF DIFFUSER

The integrating sphere of the original design of the ozonesonde has been replaced with a diffuser plate. Two types of diffuser assemblies have been used. One is made up of three pieces of ground fused silica cemented together. The other is a barium sulfate coated fused silica plate. The transmittance of the diffusers was measured on the 0 to 10%T range with a neutral density screen of approximately 1%T in the reference beam. The spectra were scanned at 2.5 Å/sec from 3425 to 2500 Å; the full slit height was used. Data were recorded every angstrom.

IV. CALCULATION OF FILTER TRANSMITTANCE FUNCTION $F(\lambda)$

The purpose of this section is to describe the methods used in the computer programs to transfer data from a record on punched paper tape and to compute numerical quantities characterizing the filter transmittance, $F_j(\lambda)$.

The programs were coded in FORTRAN V and FLECS.* The plotting routines all use the Integrated Graphics System and the FR-80 plotter by means of the Naval Weapons Center (NWC) subroutine CURVEG or PLOTSG.⁶

* FLECS (Fortran language with extended central structures).⁵

⁵ Terry Beyer. *FLECS: User's Manual*, Computing Center, University of Oregon.

⁶ Naval Weapons Center. *User Oriented Computer Graphics With Subroutine PLOTSG, CURVEG, and SHOMAT*, by Alan L. Craig and C. Howard Shomate. China Lake, Calif., NWC, March 1972. 90 pp. (NWC Technical Note 404-133, publication UNCLASSIFIED.)

The programs are on disc storage at NWC under the qualifier "ROCOZ", with file names TAPECARD, EDIT, and OFFSET. The names of the elements in each file are given in Appendix B.

The process of obtaining the F_j is broken into several stages to permit evaluation and convenient editing of the original data. This method also allows modifications for observing the effects of variations. As a result, the method is not an efficient production model, nor is it intended to be.

A complete data run is made up of the following four programs, each of which will be discussed separately: the TAPECARD program which transfers spectrophotometric data from punched paper tape to punched cards; the EDIT program which checks the cards for bad punches, ordering of wavelengths, and duplicate or missing data; the OFFSET program which applies an offset correction, smooths the 100% line, and calculates percent transmittance (the F_j 's); and the ALPHAEFF program which computes the effective ozone absorption coefficient. This section (IV) describes the first three computer programs.

A. TAPE-TO-CARD PROGRAM, TAPECARD

The TAPECARD program converts the information on punched paper tape to data punched on cards. The tape is read on a PDP-11 computer into a named storage file in the UNIVAC 1110 computer, where data are stored in PDP form. Each character is scanned and converted from paper tape code to punched card code. When 80 characters have been scanned, a line is printed and a card is punched. The pattern of numbers on the tape is:

$\backslash sxx\backslash xxxxxx$, where \backslash is a blank, x is a digit, and s is either a digit or the symbol #.

A full line of printed output consists of eight of these patterns. If a space does not occur where it should, the scan for that 80 characters stops and a new scan commences. When this happens the punched card and printed output correspondingly will have only a partial line, followed by a new line. In this way, the transmittance-wavelength pairs are aligned making these errors obvious on the printed page. Subsequent card corrections are also easier to make.

An example of a card deck used to command the UNIVAC 1110 computer to print and punch the data received from the PDP-11 computer is shown in Figure 1. The only changing quantities in the card deck are the names of the punched paper tapes. The tape name begins in column 1 and uses no more than six characters. The tape name is followed by a period and TAP. There must be no blanks between column 1 and P of TAP. Example: For a tape named MEH1, the tape name card would read

MEH1.TAP .

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```
@RUN  026PCH . . .
@ASG,A 3130131*PDPPSEUDO001.
@ASG,AX ROCOZ*TAPECARD.
@XQT  ROCOZ*TAPECARD.PCH
MEH1.TAP
MEH2.TAP
.
.
.
.
@FIN
```

FIGURE 1. Deck Structure for the TAPECARD Program.

B. EDIT PROGRAM

The EDIT program takes raw data in the form of punched cards from the TAPECARD program, edits them for bad punches and sequencing, interprets coded data, and tabulates and plots the data.

Each data card from the TAPECARD program contains eight transmittance-wavelength pairs in fields of 10. A typical card for the 100% line may contain, for example, after a first blank, the sequence

```
998 03363 #01 03362 #01 03361 999 03360 #03 03359
#02 03358 #05 03357 #02 03356 #04 03355 #05 03354
```

which corresponds to transmittance value (in digital counts) 998 for wavelength 3363, and transmittance 1001 for wavelength 3362. The "#" sign is a code on the punched paper tape which is changed by the EDIT program to the two digits, 10. The program searches for the beginning wavelength 3399 Å among the first five cards (stopping if it does not find the wavelength). Then it checks whether the wavelengths are in descending order beginning with 3399 Å and ending at or before 2500 Å. The wavelength and its corresponding transmittance value are stored in arrays IX and Y. The last card must contain a wavelength ≥ 2500 Å. While the program checks that the wavelengths are in descending order, it also checks that transmittance values (e.g., #13) contain the proper characters for the position, and whether any wavelengths are duplicated or missing. In case of an error, an appropriate message with identifying wavelength is printed, and in the case of an improperly formatted transmittance value, a value almost equal to the lower limit of the plotting scale is substituted, so that the error shows up dramatically on the plot (see Figure 2). If twenty errors are found, the program stops. After wavelength 2500 Å has been reached, the wavelength-transmittance value pairs are printed and plotted.

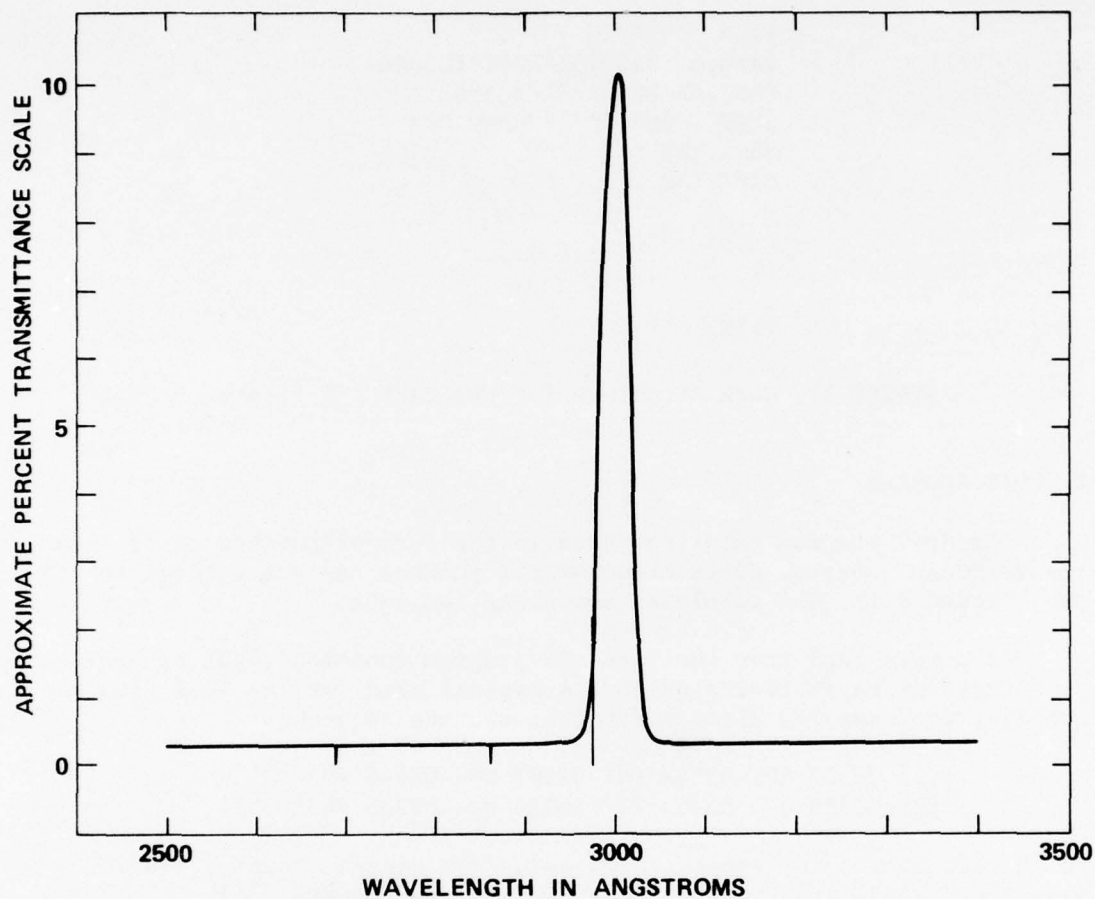


FIGURE 2. Plot of Raw Data by the EDIT Program for the $J = 1$ Filter of the LD-14 Filter Assembly. The ordinate scale is approximate because the zero offset and the 100% line deviations have not been corrected for. The three points with zero value represent bad data.

The EDIT program treats many sets of data identically. Each set requires an identifying number and designation of the spectrophotometer range used during the recording of data in order for the program to position the decimal point correctly in the transmittance data. The identifying number of the spectrum is punched out by the TAPECARD program at the beginning of the transmittance data.

An example of the card deck used to run the EDIT program is given in Figure 3. There is one data deck for each spectrum; as many data decks as desired may be used.

```

@RUN 026EDT . . .
@ASG,AX ROC0Z*EDIT.
@USE H,ROC0Z*EDIT
@XQT H.MAIN
06137514080613751408
2,1,0
028 03402 028 03401 028 03400 028 03399 028 03398 028 03397 028 03396 028 03395
. . .
. . .
028 02501 028 02500 028 02499 028 02498 028 02497 028 02496 028 02495 028 02994
@EOF
06137514010613751401
3,1,0
#21 03400 #21 03399 #23 03398 #23 03397 #21 03396 #21 03395 #24 03394 #19 03393
. . .
. . .
@EOF
. . .
@FIN
  
```

Deck for
Spectrum
No. 8

ID Card →
IRANGE Card →
Data Card →

Deck for
Spectrum
No. 1

FIGURE 3. Deck Structure for the EDIT Program.

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The cards are discussed in order of their appearance.

Card 1 ID Card Format (6A6)

Cols.	Content
2-11	ID, identification number (e.g., 0522751335; this shows that the data were taken 5/22/75 for filter assembly 13, spectrum no. 35).
12-21	ID, identification number repeated (not required but usually present).

Card 2 IRANGE Card Format ()

-, -, - IRANGE, LAMDEL, NDEG (e.g., 3, 1, 0) appearing anywhere on the card and separated by two commas.

IRANGE controls the placement of the decimal in the transmittance values and the limits of the ordinate of the plot. The possible values of IRANGE are 1, 2, 3, or 4. Table 1 shows the meaning of the parameter.

TABLE 1. Values of IRANGE for the EDIT Program.

IRANGE	Cary 14R range	Ordinate range of plot	For use with
1	0 to 100%	-10 to +110%	spectrum run on 0 to 100% range
2	0 to 10%	-1 to +11%	spectrum run on 0 to 10% range
3	0 to 100%	80 to 120%	100% line data
4	0 to 100%	-5 to +5%	0% line run 0 to 100% range

LAMDEL is the interval in angstroms between recorded wavelengths. This is normally 1.

NDEG is a plotting parameter either left blank, set to zero, or set to n, in which case a curve of the nth degree is fitted to the data. In this case the parameter M in the program must be set to 8 x NP + 1000 where NP is the number of points.

Card 3 Data Card Format (80R1)

A data card contains up to eight transmittance-wavelength pairs punched by the TAPECARD program. Each pair occupies ten columns in the pattern.

bsxxbxxxxx

where b is a blank,
s is either a digit or the symbol #,
and x is a digit.

The output of the EDIT program consists of a tabulation of a running index from 1 to 900 along with corresponding wavelength and transmittance values. Statements giving wavelengths duplicated or missing are printed with the tabulation as are statements indicating the existence of nondigital values in columns which should contain digital values only. A plot of transmittance values versus wavelength is made for each spectrum (Figure 2). Erratic values show plainly on the graphical output.

The data cards are corrected as indicated by the EDIT program and are used to calculate the transmittances of the filters.

C. OFFSET PROGRAM

The OFFSET program processes seven data decks to obtain the percent transmittances for the four filters making up a given filter assembly. The first two programs, TAPECARD and EDIT, treat all the data the same, merely resulting in uncorrected data on punched paper tape being changed into corrected data on cards. In the OFFSET program, however, the data decks all belong to the same filter assembly and must be arranged (barring exceptional cases) in the following sequence.

1. 100% line deck, a reference for the subsequent decks
2. Nominal 3200 Å filter deck
3. Nominal 3000 Å filter deck
4. Nominal 2875 Å filter deck
5. Nominal 2650 Å filter deck
6. Nominal 2650 Å filter against screen B deck
7. Screen B deck.

The expression "filter A against screen B" means that the transmittance of filter A was measured with the reference beam attenuated by a neutral density screen called B. Since screen B has a transmittance of approximately 1%, the upper limit of the transmittance scale becomes about 0.1%T.

The zero of the spectrophotometer pen seldom corresponds to the zero of the pen position encoder. The difference between the zeroes of the pen and the encoder is called the offset and the term gives rise to the name of the program which corrects for it.

The OFFSET program subtracts the offset correction (an input quantity) from each point of the 100% line, smooths the line, performs the calculations necessary to produce percent transmittances for each filter band, prints, punches cards, and plots the result. The following outline describes in algorithmic form the instructions the computer receives to perform the necessary calculations.

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1. Read the offset correction ZE100 and the wavelength-transmittance data pairs for the 100% line. Call the EDIT subroutine, which edits the data (see the description for the second program, the EDIT program). Subtract the correction ZE100 from each transmittance value, Y(I), and scale by dividing by D = 10, a value which is assigned by IRANGE. Find the wavelength nearest the 2500 Å end which is a multiple of 5 and make it the last wavelength. Then count the number of wavelength-transmittance pairs, calling the total N100.

2. Call the AVRIJ subroutine to smooth the 100% line by making a sliding average of 21 points, assigning the average value to the mid-point. The processed values are called SM100(I), I = 1, N100.

(The program then moves on to obtain transmittance values corresponding to data in six decks identified by JFIL = 1, ..., 6. The processing outlined in Step 3 is identical for the first three decks but the last three decks are treated differently, as outlined in Steps 5, 6, and 7.)

3. Read the data for the filter consisting of JFIL (filter number) and NZER. NZER is the *input* offset correction for the filter and is left blank on input for filters JFIL = 1, 2, 3, 4, since it is computed in the program (see below). For JFIL = 5, 6, a nonzero offset may be input, which is used instead of the computed value.

a. Find the wavelength, LMAX, corresponding to the maximum transmittance, YMAX. If there are several LMAXs, choose the one nearest 2500 Å. The corresponding index is called IMAX.

b. Obtain the offset correction ZER near the red end of the spectrum, i.e., near 3400 Å, for J = 1 through 5. If the offset correction is input (i.e., NZER ≠ 0), do not compute ZER. If the offset correction is not input (NZER = 0), average the 50 transmittance data corresponding to 50 wavelengths beginning at the red (long wavelength) end of the spectrum, and call the integer closest to the average, ZER.

c. Average the transmittance data corresponding to the last 50 wavelengths at the blue end of the spectrum, i.e., near 2500 Å, and call the integer closest to the average value, ZEB, the offset correction for the blue (short wavelength) end of the spectrum.

d. If ZER = ZEB, the transmittance $\text{TAU}_1(I)$ is given by

$$\text{TAU}_1(I) = \frac{(\text{FJ}(I) - \text{ZER})100}{\text{SM100}(I)}, \quad I = 1, \text{NMIN} \quad (3)$$

where FJ(I) is the transmittance value for the corresponding wavelength LAM(I), SM100(I) is the value of the smoothed 100% line corresponding to wavelength LAM(I), NMIN is the smallest of the numbers 900, N100 (the number of points in the 100% line), and NN (the number of points in the filter data).

e. If $ZER \neq ZEB$, subtract ZER from each transmittance value near the 3399 Å end to $LMAX$, and subtract the blue offset value ZEB from $LMAX$ to the blue end. That is,

$$TAU_1(I) = \frac{(FJ(I) - ZER)100}{SM100(I)}, \quad I = 1 \text{ to } I_{MAX} \quad (4)$$

and

$$TAU_1(I) = \frac{(FJ(I) - ZEB)100}{SM100(I)}, \quad I = I_{MAX} + 1 \text{ to } NMIN. \quad (5)$$

f. Reorder the points so that the first wavelength $LAM(1) = 2500$.

g. Find the maximum transmittance, $YMAX$, for the corrected %Ts. Determine the wavelengths $CLAMB$ and $CLAMR$ at which the transmittance is one-half the maximum value, $YHAF = YMAX/2$. Calculate the center of the bandpass, $CLAMC$.

$$CLAMC = (CLAMB + CLAMR)/2 \quad (6)$$

Calculate the width, W , of the band at half-height.

$$W = CLAMR - CLAMB \quad (7)$$

h. Punch cards with wavelength and percent transmittance pairs for the four filters or for (2650/screen B) x screen B in a format acceptable to the ALPHA EFF program, along with the constants to be used in that program.

4. For $JFIL = 2$ and 3, treat the 3000 Å filter and the 2875 Å filter as in 3.

5. For $JFIL = 4$, the 2650 Å filter, use 3a, b, d, f, g and h. Set ZEB equal to ZER .

6. For $JFIL = 5$, the 2650 Å filter against screen B, (written 2650/s and identified as $JFIL = 5$) has only the red end of the band, and hence only ZER . Use 3a, b, d, f and g to obtain $TAU_1(I)$, which is stored for use in 7.

7. For $JFIL = 6$, for screen B, set $ZER = ZER4$ if $NZER = 0$; otherwise set $ZER = NZER$.

Calculate

$$TAU_2(I) = TAU_1(I) \frac{Y(I)ZER}{SM100(I)} \quad (8)$$

The desired transmittance for the long wavelength tail of the 2650 Å filter on the extended range is

$$TAU(I) = (TAU_1(I)TAU_2(I))100, \quad \lambda(I) > 2750 \quad (9)$$

(If either $\text{TAU}_1(I)$ or $\text{TAU}_2(I)$ is nonexistent for a particular I , the product is set to zero for that I .)

The input data decks, seven in number, are the corrected decks from the EDIT program. The input quantities are those of the EDIT program plus one card in front of each data deck to notify the OFFSET program what data deck to expect (JFIL) and to provide an offset value where necessary. ZE100 is the offset correction for the 100% line. It is a required input and is an integer. NZER is an input offset for 2650/s and screen B decks. It is not required and, if not input, the offset will be computed in the OFFSET program. It should be noted that there is a comma after ZE100 but not after NZER (see Figure 4).

An illustration of the input decks for the OFFSET program is given in Figure 4.

Figures 5 through 8 show the transmittance of the filters for LD-14 as calculated and plotted by the OFFSET program. Figure 9 shows the long wavelength tail of the 2650 Å filter on an expanded scale.

V. CALCULATION OF DIFFUSER TRANSMITTANCE FUNCTION $S(\lambda)$

The purpose of this section is to describe the computer program (called DIFFUSER) used to calculate the diffuser transmittance function from data stored on punched cards which have been edited by means of the EDIT program described in Section IVB.

The DIFFUSER program is described here because it is a modified OFFSET program and in its logic the DIFFUSER program follows the OFFSET algorithm. However, there are only three input data decks instead of seven. They are (1) the 100% line deck; (2) diffuser against screen B deck (JFIL = 5); and (3) screen B deck (JFIL = 6).

The input quantities are ZE100 and NZER as in the OFFSET program. In distinction to the OFFSET program, NZER is a required input to the DIFFUSER program. An illustration of the input decks for the program is given in Figure 10.

The output of the program is a tabulation of the input and output data, a plot of diffuser transmittance versus wavelength, and a deck of punched cards containing the diffuser transmittance in the format required by the ALPHA EFF program. It should be noted that although the calculated values are referred to as transmittance the term is not used in its usual sense as the spectrophotometer is designed to measure the transmittance of nonscattering samples and the diffusers are highly scattering. Figure 11 shows the transmittance of a BaSO_4 coated type diffuser and Figure 12 shows the transmittance of a ground, fused silica type diffuser. The DIFFUSER file is listed in Appendix B.

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```

@RUN 0260FS . . .
@ASG,AX ROCOZ*OFFSET.
@USE R,ROCOZ*OFFSET
@XQT R.MAIN
100,26,
06137514010613751401
3,1,0
Deck for { #21 03400 #21 03399 #23 03398 #23 03397 #21 03396 #21 03395 #24 03394 #19 03393
100% {
Line {
.
.
.
.
#21 02503 #24 02502 #24 02501 #24 02500 #23 02499 #24 02498 #24 02497 #23 02496
@EOF
1,
06137514030613751403
2,1,0
JFIL = 1 { 028 03402 028 03401 028 03400 028 03399 028 03398 028 03397 028 03396 028 03395
(3200 Å) {
.
.
.
.
@EOF
2,
JFIL = 2 {
(3000 Å) {
.
.
.
.
@EOF
3,
JFIL = 3 {
(2880 Å) {
.
.
.
.
@EOF
4,
JFIL = 4 {
(2630 Å) {
.
.
.
.
@EOF
5,
JFIL = 5 {
(2630 Å/S) {
.
.
.
.
@EOF
6,29
JFIL = 6 {
(Screen) {
.
.
.
.
@EOF
@FIN

```

FIGURE 4. Deck Structure for the OFFSET Program.

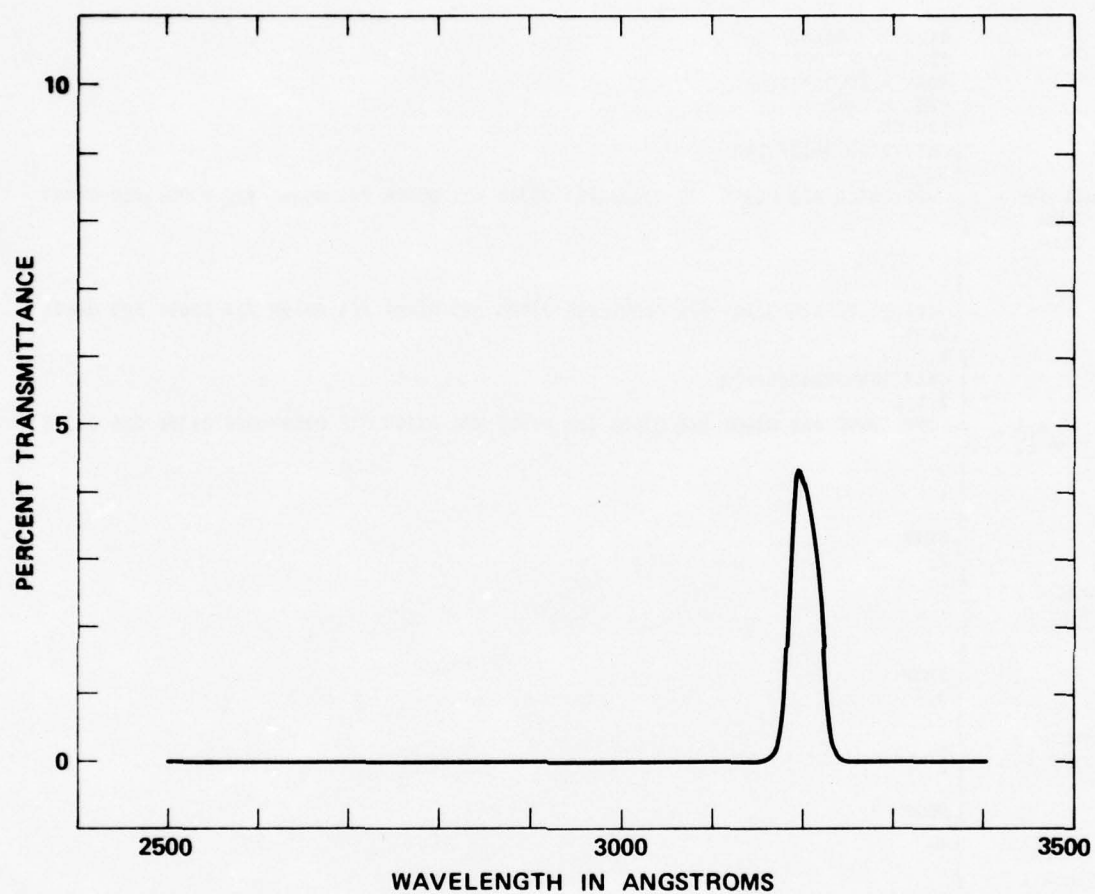


FIGURE 5. Transmittance of the J = 0 Filter of the LD-14 Filter Assembly.

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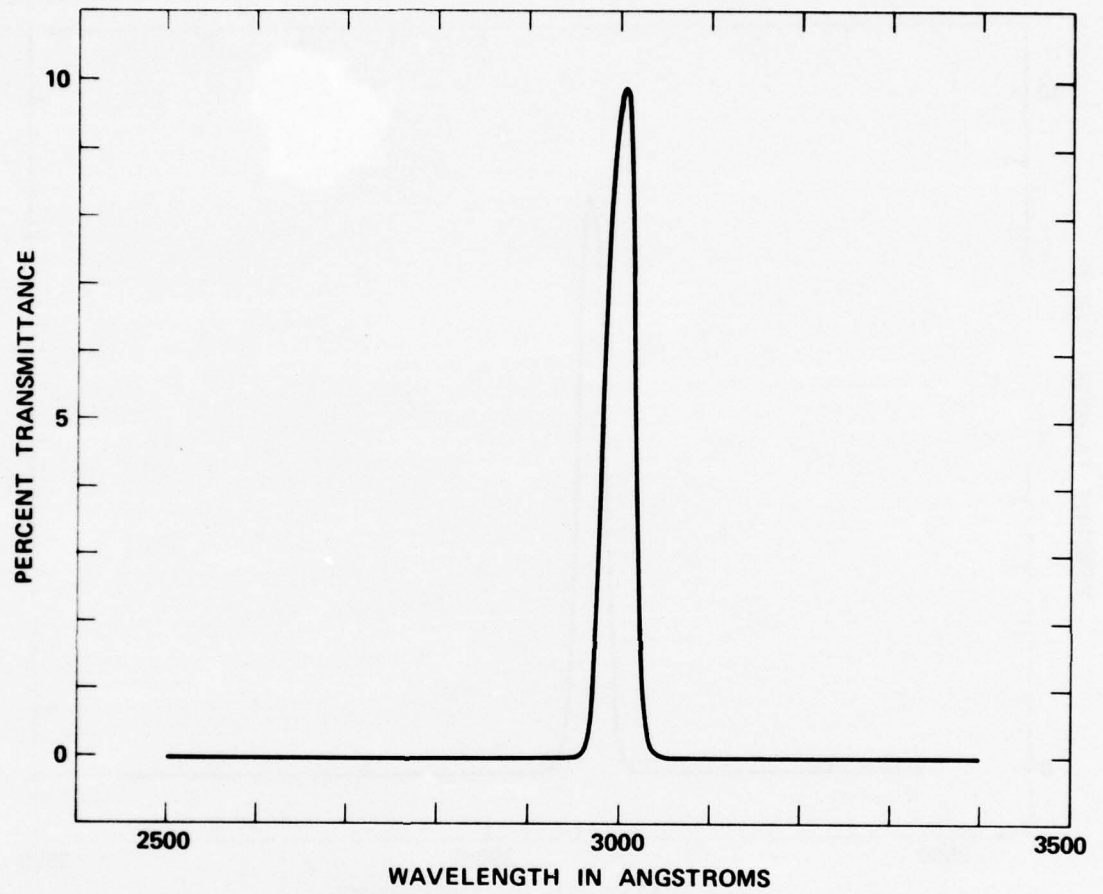


FIGURE 6. Transmittance of the J = 1 Filter of the LD-14 Filter Assembly.

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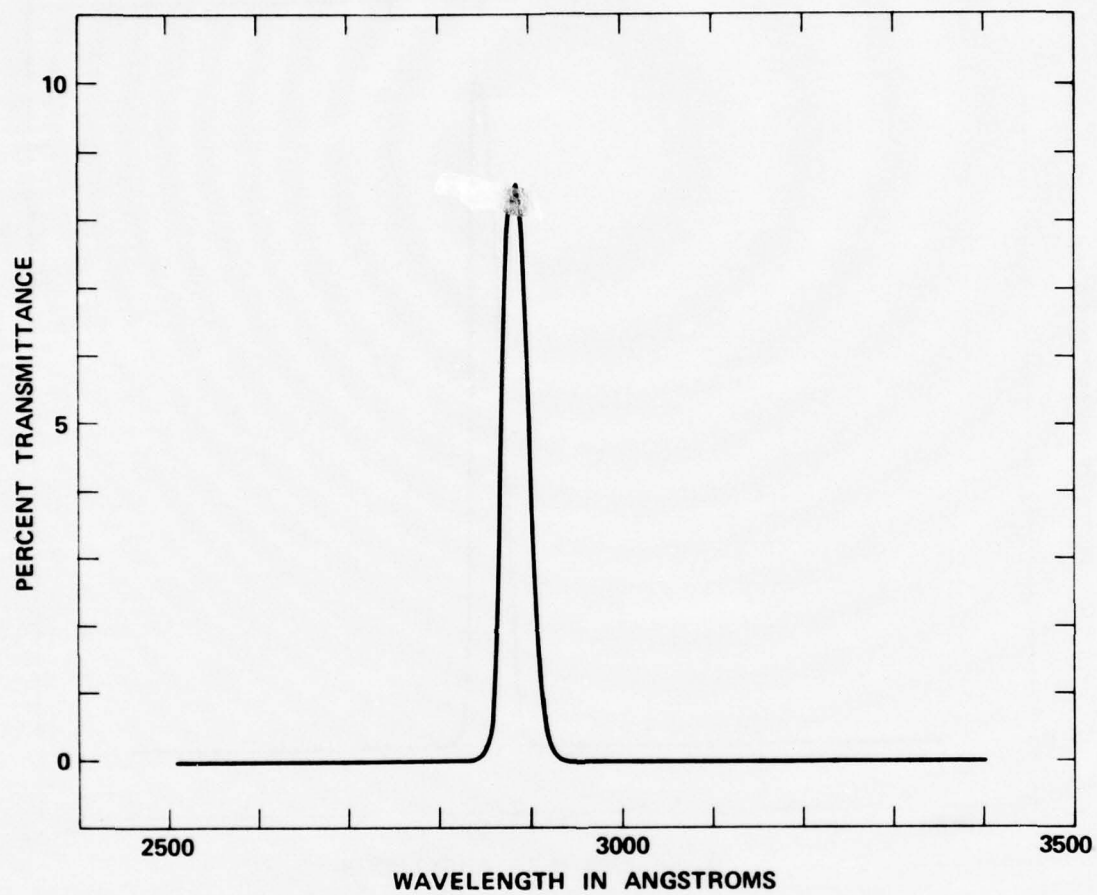


FIGURE 7. Transmittance of the J = 2 Filter of the LD-14 Filter Assembly.

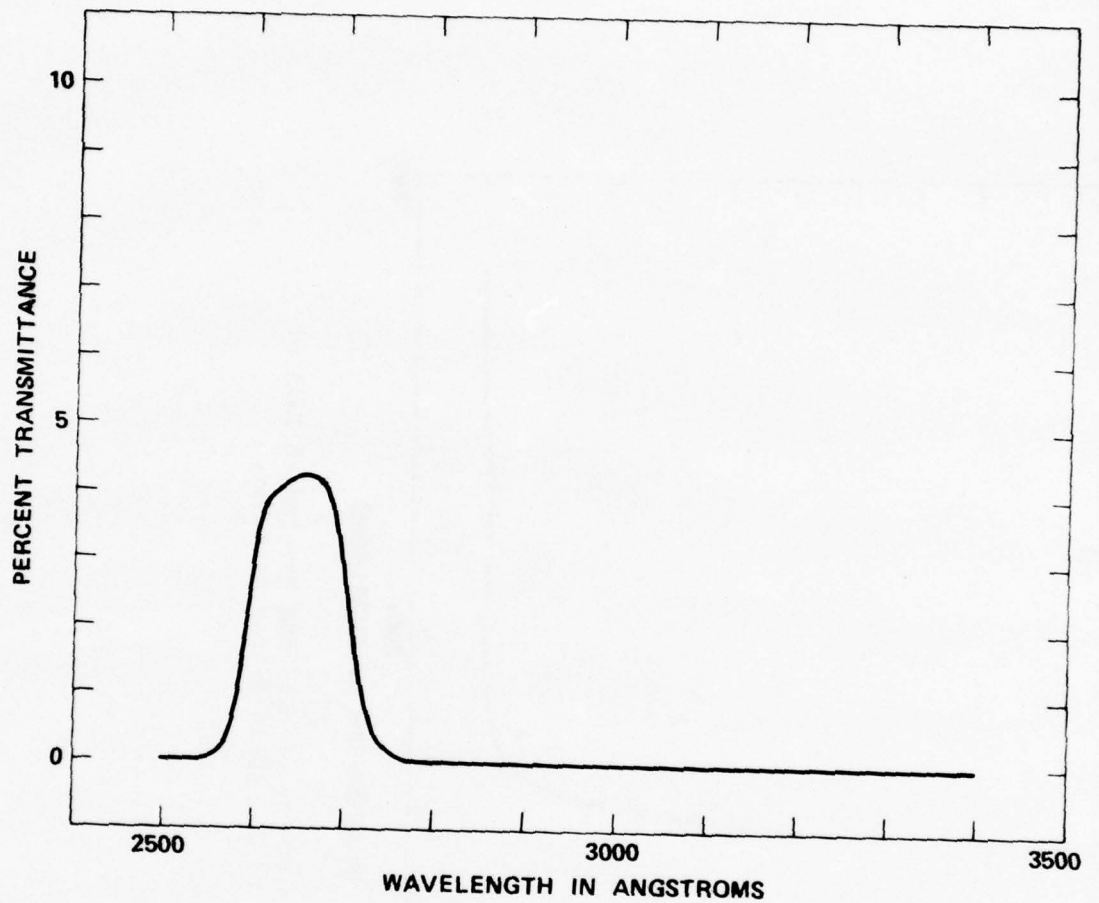


FIGURE 8. Transmittance of the J = 3 Filter of the LD-14 Filter Assembly.

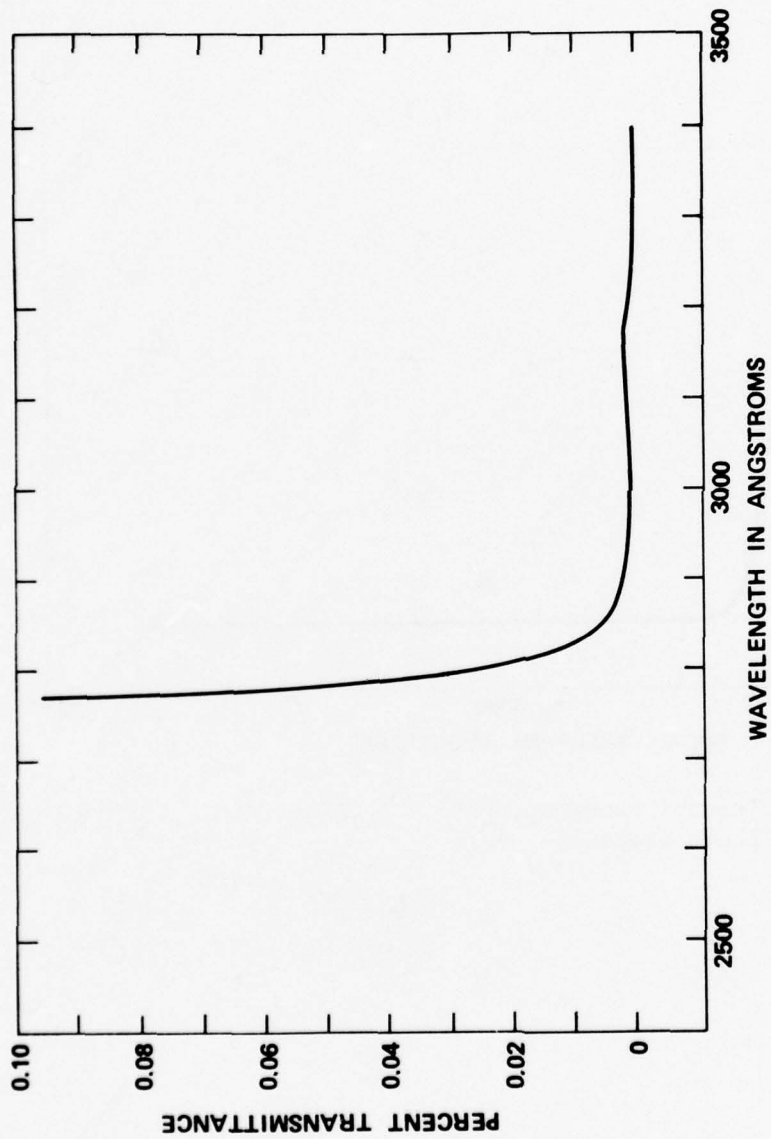


FIGURE 9. Transmittance of the Long Wavelength Tail of the J = 3 Filter of the LD-14 Filter Assembly.


```

@RUN 026DIF . . .
@ASG,AX ROCOZ*DIFFUSER.
@USE R,ROCOZ*DIFFUSER
@XQT R.MAIN
{
100,34,
06277600010627760001
3,1,0
#32 03401 #32 03400 #32 03399 #31 03398 #35 03397 #31 03396 #31 03395 #32 03394
.
.
.
#35 02505 #38 02504 #36 02503 #36 02502 #36 02501 #35 02500 #34 02499 #36 02498
} @EOF
5,34
06277600020627760002
2,1,0
722 03400 720 03399 719 03398 716 03397 716 03396 717 03395 717 03394 716 03393
.
.
.
} @EOF
6,33
06277600030627760003
2,1,0
364 03404 361 03403 363 03402 362 03401 361 03400 361 03399 362 03398 362 03397
.
.
.
} @EOF
@FIN

```

100%
Line

Diffuser

Screen

FIGURE 10. Deck Structure for the DIFFUSER Program.

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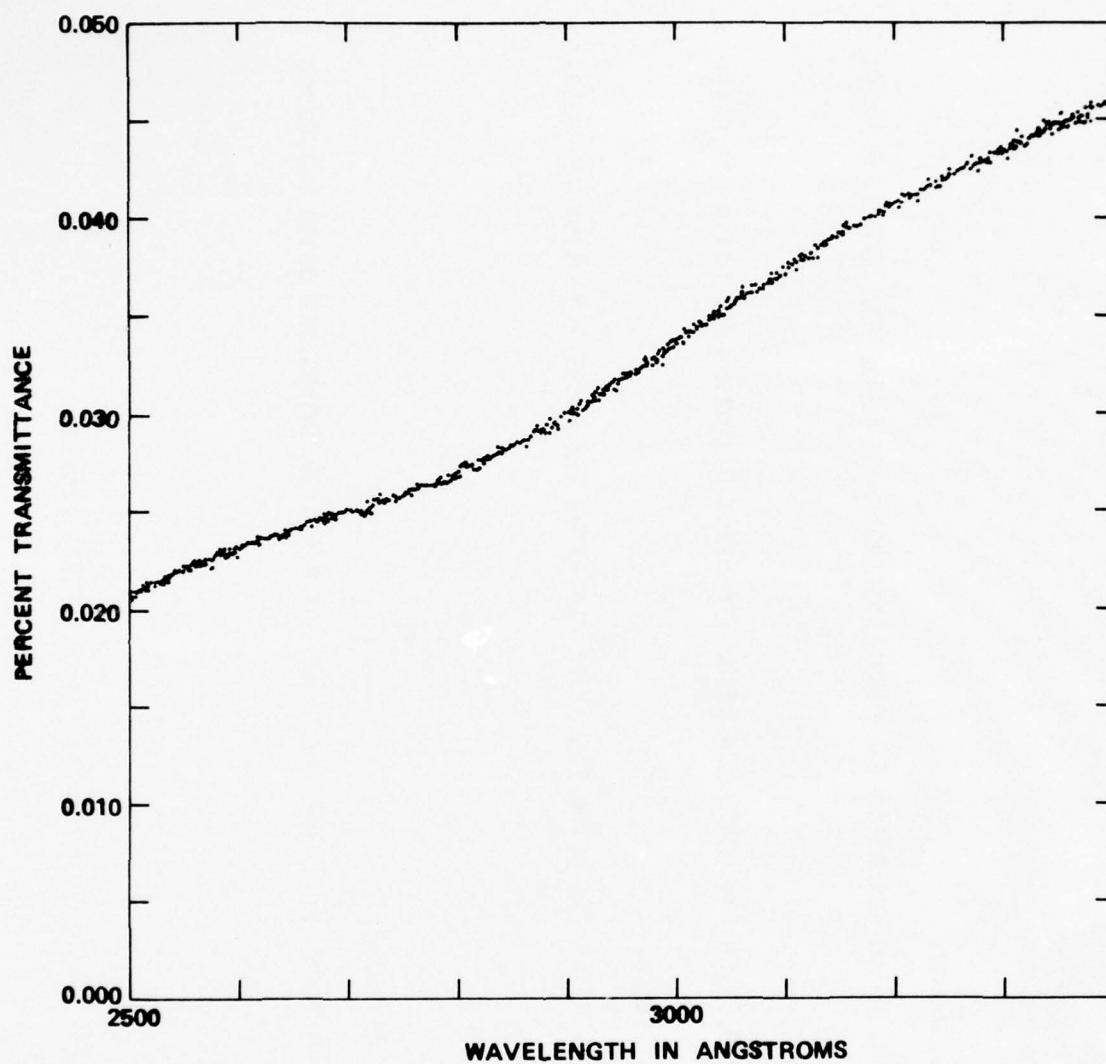


FIGURE 11. Transmittance of a Barium Sulfate Coated Diffuser Assembly.

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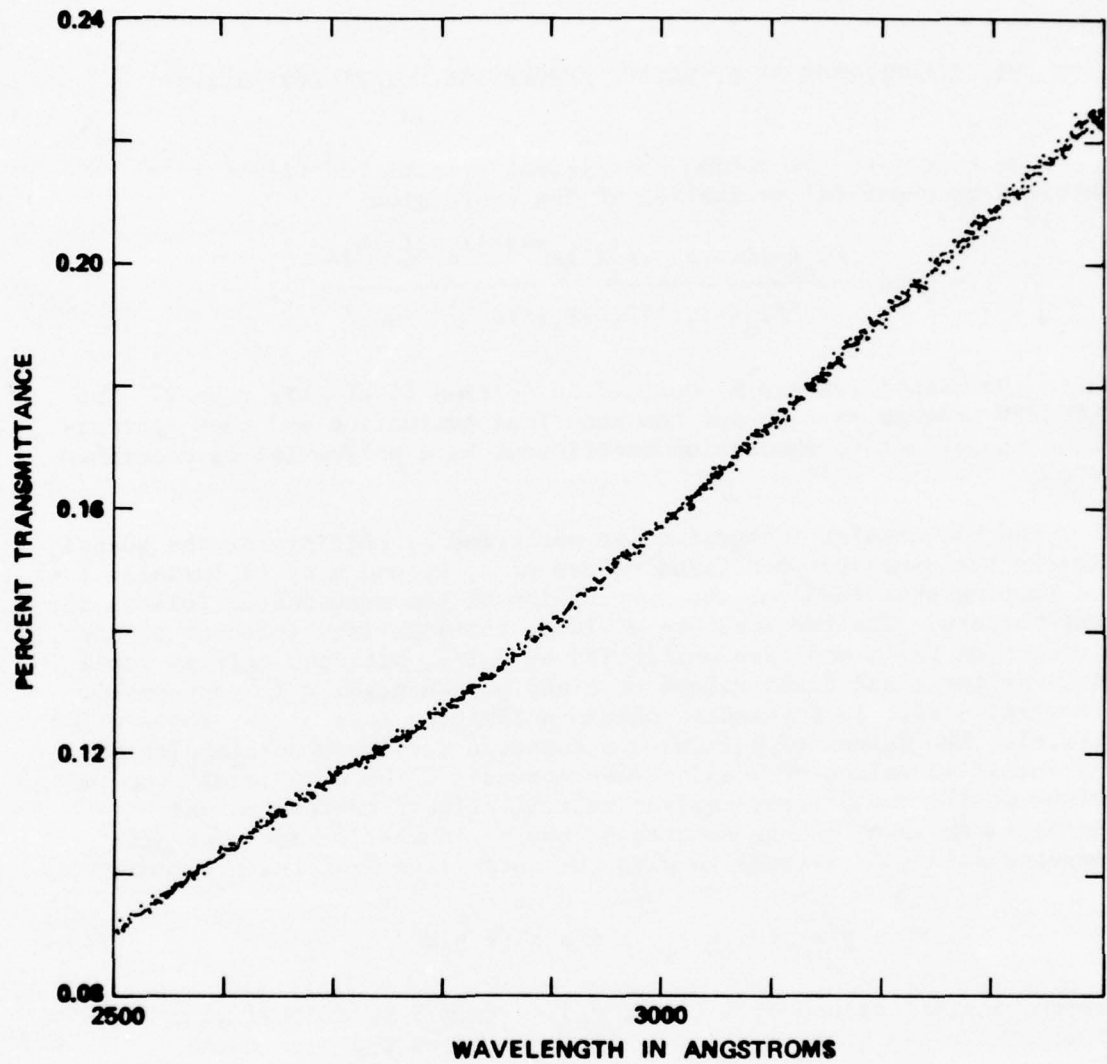


FIGURE 12. Transmittance of a Quartz Diffuser Assembly.

VI. CALCULATION OF EFFECTIVE ABSORPTION COEFFICIENT $\alpha(x, m)$

The effective absorption coefficient $\alpha_j(x, m)$ for filter j is obtained by numerical evaluation of the expression

$$-\frac{1}{x} \ln \frac{\int I_0(\lambda) Q(\lambda) S(\lambda) F_j(\lambda) e^{-\alpha(\lambda)x} e^{-\beta(\lambda)m} d\lambda}{\int I_0(\lambda) Q(\lambda) S(\lambda) F_j(\lambda) e^{-\beta(\lambda)m} d\lambda},$$

where the quantities are as defined in Section II of this report. The ALPHAEFF program carries out the numerical evaluation and then approximates the effective absorption coefficient by a polynomial as described below.

The rectangular integration is performed by multiplying the quantities in the numerator for fixed values of λ , x , and m by $\Delta\lambda$ (usually 1 Å) and summing over the λ 's; the computation of the denominator follows the same pattern. The two sums are divided, the logarithm (base e) of the dividend is taken and then multiplied by $-1/x$, yielding $\alpha_j(x, m)$ for a given filter j and fixed values of x and m . Whenever x is very small, l'Hôpital's rule is invoked to obtain a limiting form of the formula for $\alpha_j(x, m)$. The values of $\alpha_j(x, m)$ are computed for every combination of the specified values of x and m (see Appendix C for a table of x and m values used), and a least-squares multiple-linear-regression which minimizes the sums of the squares of the residuals is made over all computed values of $\alpha_j(x, m)$ to give the coefficients of the polynomial

$$P_j(x, m) = a_0 + a_1 x + b_1 m + a_2 x^2 + b_2 m^2. \quad (10)$$

For the initial values of m (i.e., m_0), $\alpha_j(x, m_0)$ is plotted as a function of x ; the values of $P_j(x, m_0)$ are also plotted on the same graph.

Since the assembly of the cards and data decks used in the ALPHAEFF program is more complex than for the other programs, the process will be described in greater detail than was done for the other programs.

All of the input parameters for the ALPHAEFF program are punched out by the OFFSET program. The input quantities $I_0(\lambda)$, $Q(\lambda)$, $S(\lambda)$, $\alpha(\lambda)$, and $\beta(\lambda)$ are stored on a disc and called up for use by the @ADD control cards. Figure 13 is an illustration of an assembled ALPHAEFF deck.

The parameter cards punched by the OFFSET program will be discussed in the order of their appearance in the assembled ALPHAEFF deck.

Card 1	λ -Parameter Card	Format (4F5.0, 5X, 11)
<u>Cols.</u>		<u>Content</u>
1-5		ALAMO, the beginning wavelength, e.g., 2500 Å.
6-10		ALAMF, the ending wavelength, e.g., 3399 Å.
11-15		DELLAM, the interval between wavelengths, usually 1.
16-20		AK, a scaling factor for the numerator integrand, usually 1.
26		NFLTRS, the number of filters being processed, usually 4.
Card 2	Title Card	Format (4A5, 15)
<u>Cols.</u>		<u>Content</u>
2-19		Title, e.g., LOKI DART 12.
25		Diffuser number, e.g., 4.
Card 3	x-Parameter Card	Format (I5, 2F10.1, F5.0, F5.3, I5, F5.0)
<u>Cols.</u>		<u>Content</u>
1-5		J, filter number.*
6-15		CLAMC, center of the bandpass.
16-25		W, width of band at half-height.
26-30		XINT, initial x value, usually 0.
31-35		DELX, the interval between x values (.05, .02, .005, .001 for filters 0 to 3, respectively, are in current use).
26-40		NXS, the number of x's to be computed (12, 24, 20, 20 currently in use).
40-45		XFACT0, a scaling factor for the x's (currently XFACT0 = 1).

* J, the filter number. On input J = 1, 2, 3, 4; on output J = 0, 1, 2, 3, chiefly for historical reasons.

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Card 4 Identification Card Format (10A6)

<u>Cols.</u>	<u>Content</u>
2-11	ID number, e.g., 0522751335.
12-21	ID number, repeated.

Card 5 m-Parameter Card Format (2F10.0, I5, F10.0)

<u>Cols</u>	<u>Content</u>
10	m ₀ , initial value for m, usually zero.
11-20	DELM, the interval between computed values of m. (The values .2, .2, .01, .01 are currently used for filters 0 to 3, respectively.)
24,25	NMS, the number of m's to be computed (10, 10, 05, 05 currently in use).
26-35	FACTRM, a scaling factor for the m's (currently FACTRM = 1).

Card 6 MLR-Parameter Card Format (5I3, 2F4.0)

<u>Cols.</u>	<u>Content</u> [*]
1-3	ITEST, the test case number (0).
4-6	N, the number of observations (0).
7-9	NPl, the number of independent and dependent variables (5).
10-12	IW, weighting factor indicator (0).
13-15	LIMIT, the maximum number of steps in the regression analysis (5).
16-19	EFIN, the F value for entering a variable from the regression (2.5).
20-23	EFOUT, the F value for removing a variable from the regression (2.5).

Four decks from the OFFSET program, one for each filter of the filter assembly, form the core of the ALPHAEFF deck.

Except for two beginning and two ending cards, the data decks punched by the OFFSET program consist of transmittance-wavelength pairs punched five to a card, beginning with a wavelength near 2500 Å which is a multiple of 5 and continuing in ascending order no further than 3399 Å. These cards are easily distinguished from the original data cards (which were in descending order beginning with 3399 Å and punched eight pairs to a card).

* Values of the parameter currently being used are entered in parentheses.

```

@RUN 026ALF . . .
@ASG,AX ROCOZ*ALPHA EFF.
@USE P,ROCOZ*ALPHA EFF
@XQT P.MAIN
2500.3399. 1. 1. 4
@ADD,P P.IO
@ADD,P P.Q
@ADD,P P.ALPHA
@ADD,P P.BETA
LOKI DART 14
@ADD,P P.S
1 3200.0 37.7 0. .050 12 1.
x-Parameter Card →
ID Card → 06137514030613751403
Data Card → .000 2500. .000 2501. .000 2502. .000 2503. .000 2504.
.
.
.000 3395. .000 3396. .000 3397. .000 3398. .000 3399.
@EOF
m-Parameter Card →
MLR Parameter Card → 1 0. .20 10 1.
2 2999.3 36.3 0. .020 24 1.
3 2879.2 32.9 0. .005 20 1.
.
.
.000 3395. .000 3396. .000 3397. .000 3398. .000 3399.
@EOF
J = 2
(3000 Å)
J = 3
(2880 Å)
J = 4
(2630 Å)
1 0. .01 5 1.
5 5 2.5 2.5
4 2651.1 113.2 0. .001 20 1.
.
.
@FIN

```

FIGURE 13. Deck Structure for the ALPHA EFF Program.

If noise in the tails of the transmittance bands was not removed previously, it is removed at this time by replacing the cards having nonzero transmittance values with blank cards in wavelength ranges where it is obvious that the transmittance should be zero. Since the ALPHAEFF program does not read the wavelengths, blank cards may be used. This does away with the necessity to punch cards and for this reason it is easier to remove noise at this point rather than earlier.

Before the data cards are used in the ALPHAEFF program, it is necessary to replace part of the cards in 2650 Å filter deck with cards from the transmittance measurements made with a neutral density screen in the reference beam of the spectrophotometer. The latter set will be called the "expanded tail" set. The crossover from normal tail to "expanded tail" is made near 0.09%T.

An end-of-file card, @EOF, signals the end of the data for a particular filter.

The output of the ALPHAEFF program consists of tabulations and plots. The following tabulations are produced.

1. List of the input data.
2. List of the values of the numerator integrand for $m = 0$ and several values of x (except for the 3200 Å filter).
3. Tabulation of x, m and the corresponding values of $\alpha_j(x, m)$.
4. Listing of the input parameters to the multiple-linear-regression program.
5. Tabulation of the approximating polynomial coefficients for each iteration until a satisfactory F-test is obtained.
6. Tabulation of $P_j(x, m)$ together with the corresponding values of $\alpha_j(x, m)$.

Figure 14 shows the tabulation of approximating polynomial coefficients for the $J = 1$ filter (nominal 3000 Å filter) of LD-14.

The plots are of two kinds.

1. Plots of the numerator integrand versus wavelength for optical depths approximately equal to 0, 1, 2, 3, and 4 (except for the 3200 Å filter). The optical depth τ is given by the expression

$$\tau = x \cdot \alpha_j(x, m). \quad (11)$$

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Step No. 3

Variable Entering 3
 Flevel 3607.594818
 Standard Error of Y .001168
 Constant 9.500789

Variable	Coefficient	Std Error of Coeff
X 1	-1.48664	.00210
X 2	-.04167	.00013
X 3	.26491	.00441

Step No. 4

Variable Entering 4
 Flevel 5.645376
 Standard Error of Y .001157 (σ_y)
 Constant 9.500496 (a_0)

Variable	Coefficient	Std Error of Coeff
X 1	-1.48664 (a_1)	.00208
X 2	-.04058 (b_1)	.00048
X 3	.26491 (a_2)	.00437
X 4	-.00061 (b_2)	.00026

FIGURE 14. A Representation of the Computer Printout Showing Results for the Last Two Iterations in the Determination of the Coefficients of the Polynomial $P_1(x,m) = a_0 + a_1x + b_1m + a_2x^2 + b_2m^2$. The labels in parentheses are not part of the printout but were added to the representation to assist in its interpretation.

2. Plots of the effective absorption coefficient $\alpha_j(x,m)$ and its polynomial approximation $P_j(x,m)$ against the amount of ozone x for the $m = 0$ case. Figure 15 is an example of the second kind of plot.

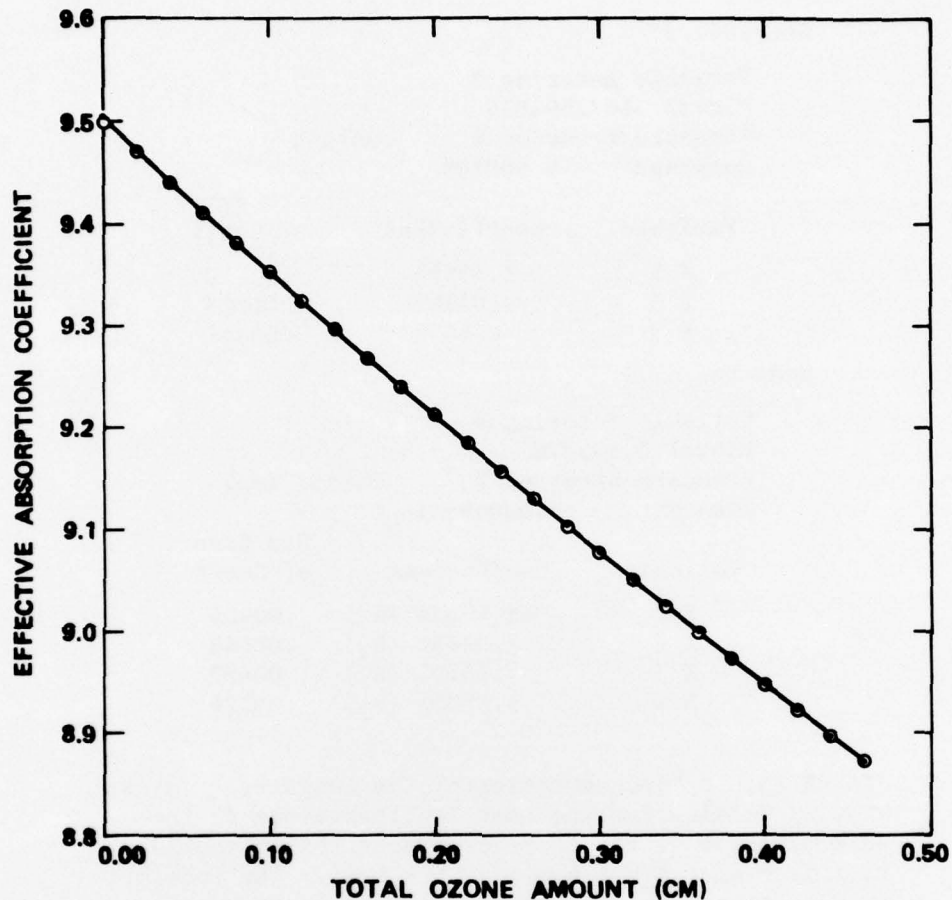


FIGURE 15. Effective Absorption Coefficient for the $J = 1$ Filter of the LD-14 Filter Assembly for the Case $m = 0$. The calculated values of $\alpha_1(x,0)$ are given by dots. The corresponding values for the polynomial are represented by circles.

VII. SUMMARY AND COMMENTS

The measurement techniques and computer programs described in this report have been used to calculate the effective ozone absorption coefficient $\alpha_j(x,m)$ and the coefficients of its polynomial approximation $P_j(x,m)$ for each of the four filters of the seventeen filter assemblies. Several diffusers have also been measured and their transmittances calculated. All but one of the filter assemblies have been flown in payloads carried aloft by Super Loki Dart rockets; the polynomials have been used by NASA to calculate ozone concentrations from the flight data.

It is anticipated that the programs will be used to calculate the polynomial coefficients for 20 to 25 additional filter assemblies forming a more homogeneous group than the first seventeen. Filter parameters, such as bandpass position (midpoint between the half-power points) and bandwidth, will be tested to see whether they may be used to calculate the polynomial coefficients for a filter assembly provided that the polynomial coefficients are known for one assembly of the group or batch. Plots of the constant term a_0 of expression (10) against the bandpass position have indicated that a_0 is related to bandpass position. A similar plot for the a_1 coefficient did not lead to any obvious relationship.

Appendix A

TAPE PUNCH CODE AND RECORD FORMATS

TABLE A-1. Tape Punch Code (IBM Odd Parity Code).

Character	Channel number/identity								
	8	7	6	5	4	o	3	2	1
	EL	X	0	CH	8	o	4	2	1
0			x			o			
1						o			x
2						o		x	
3				x		o		x	x
4						o	x		
5				x		o	x		x
6				x		o	x	x	
7						o	x	x	x
8					x	o			
9				x	x	o			x
#					x	o		x	x
-		x				o			
CR		x		x	x	o	x	x	
SPACE				x		o			
EOA	x					o			
x = Hole in tape o = Feed hole									

TABLE A-2. Identification Number Record Format

Frame	Data recorded	
1	0-9	Identification number (parameter switch settings)
2	0-9	
3	0-9	
4	0-9	
5	0-9	
6	0-9	
7	0-9	
8	0-9	
9	0-9	
10	0-9	
11	EOA	
12	CR	

TABLE A-3. Transmittance-Wavelength Data Record Format

Frame	Data recorded	
1	Space	
2	# (Ordinate ^a values above 1000) or - (Ordinate ^a values below zero) or Hundreds decade ordinate value (0-9)	
3	Tens	Ordinate ^a value
4	Units	
5	Space	
6	TTH	Wavelength (abscissa) value
7	TH	
8	H	
9	T	
10	U	
11	CR	

^a Transmittance without regard to the decimal point.

Appendix B

NAMES OF ELEMENTS IN PROGRAM FILES

1. TAPECARD FILE

The TAPECARD program is filed under ROCOZ*TAPECARD with the following element names:

- FOR PCH - This main symbolic program is coded in FLECS.
- FOR PCHFOR - The FORTRAN version of the above program, PCH.
- REL PCHFOR - The relative program for PCH.
- ABS PCH - The absolute PCH program.
- MAP SYM - The symbolic input for the MAP processor.

2. EDIT FILE

The EDIT program is filed under ROCOZ*EDIT and contains the following elements:

- MAIN - The main program orders events, calls subroutines, reads, and writes.
- SETP - This subroutine sets the parameters for plotting.

The system subroutine PLT*PLOTS\$LIBRARY must be included in the MAP to provide for plotting.

3. OFFSET FILE

The OFFSET program is filed under ROCOZ*OFFSET with the following element names:

- MAIN - The main symbolic program orders events, reads input, and prints and punches results.
- EDIT - Edits the data.
- AVRIJ - Performs a 21-point running average.
- ORDER - Reorders the data so that the first data point consists of the wavelength nearest 2500 Å, along with the corresponding transmittance data.
- PLOT - Plots the data.
- SETP - Sets parameters used in plotting.
- MAP - Contains the names of files and elements which must be collected to run the program.

4. DIFFUSER FILE

The DIFFUSER program is filed under ROCOZ*DIFFUSER and contains elements having the same names as those in the OFFSET file.

5. ALPHAEFF FILE

The ALPHAEFF program is filed under ROCOZ*ALPHAEFF and contains the following elements:

- MAIN - The main program which calls the subroutines, reads and writes. It calls PLOTIN for plotting the ALPHAEFF function and the polynomial function against x for $m = m_0$, $J = 0, 1, 2, 3$. Additionally, it calls PLOTIN to plot the numerator of the integrand of the ALPHAEFF function against λ for $m = m_0$, $OPDEP \cong 0, 1, 2, 3, 4$, and $J = 1, 2, 3$, where $OPDEP$ is "optical depth" defined as $\alpha_{eff}(x,m)$ multiplied by x .
- MRL - A subroutine which calls the RESTEM subroutine, furnishes the parameters, and prints the results.
- *RESTEM - A subroutine which performs a multiple-linear-regression on values furnished by $\alpha_{eff}(x,m)$ to fit a polynomial $P = a_0 + a_1x + b_1m + a_2x^2 + b_2m^2$. RESTEM is called by MLR.
- PLOTIN - A subroutine which plots. It is called either by MAIN or by TRY.
- IO(λ) - A data element giving extraterrestrial solar irradiance as a function of wavelength λ , $\lambda = 2500$ to 3399 \AA .
- Q(λ) - A data element for photodetector response for 900 values of λ , $\lambda = 2500$ to 3399 \AA . This element is replaced whenever the photodetector characteristic is changed.
- S(λ) - A data element providing transmittance values for the diffuser for 900 values of λ , $\lambda = 2500$ to 3399 \AA . This element is replaced whenever the type of diffuser is changed.
- ALPHA(λ) - A data element providing absorption coefficients for 900 values of λ , $\lambda = 2500$ to 3399 \AA .
- BETA(λ) - A data element providing Rayleigh extinction coefficients for 900 values of λ , $\lambda = 2500$ to 3399 \AA .
- MAP(λ) - A symbolic element giving the names of the files which need to be collected for this program.

* RESTEM is a subroutine from UNIVAC's STAT-PACK,⁷ UP-7502, Rev. 2.

⁷ Sperry Rand Corporation. UNIVAC Large Scale Systems, STAT-PACK Programmer Reference, UP-7502, Rev. 1, November 1973.

Appendix C

DISCRETE VALUES OF x , OZONE AMOUNTS, AND m , AIR MASS, USED IN
CALCULATION OF $\alpha(x,m)$, THE EFFECTIVE ABSORPTION COEFFICIENT

Filter	x , Ozone amount			m , Air mass		
	Size of increment DELX	No. of values used, NXS	Range of x	Size of increment DELM	No. of values used, NMS	Range of m
$J = 0$ (3200 Å)	0.05	12	0-0.55	0.2	10	0-1.8
$J = 1$ (3000 Å)	0.02	24	0-0.46	0.2	10	0-1.8
$J = 2$ (2880 Å)	0.005	20	0-0.095	0.01	5	0-0.04
$J = 3$ (2630 Å)	0.001	20	0-0.019	0.01	5	0-0.04

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- 1 Air Force Rocket Propulsion Laboratory, Edwards Air Force Base
- 1 2nd Weather Squadron, Andrews Air Force Base
- 12 Defense Documentation Center
 - 1 Bureau of Mines, Pittsburgh, PA (Reports Librarian)
 - 1 Lewis Research Center (Technical Library)
- 7 National Aeronautics and Space Administration, Goddard Space Flight Center, Greenbelt, MD
 - Code 900, W. Bandeen (1)
 - Code 901, E. Neal (1)
 - Code 912
 - Donald F. Heath (1)
 - E. Hilsenrath (1)
 - David Wright (1)
 - L. Dunkelman (1)
 - Carol Fry (1)
- 4 National Aeronautics and Space Administration, Wallops Flight Center, Wallops Island, VA
 - George Foster (1)
 - Charles Marion (2)
 - Thomas Perry (1)
- 1 National Oceanic and Atmospheric Administration, Environmental Research Laboratory, Boulder CO (W. D. Komhyr)
- 1 National Oceanic and Atmospheric Administration (Upper Atmosphere Branch)
- 1 Aerojet-Liquid Rocket Company, Sacramento, CA (Technical Library), via AFPRO
- 1 Aerojet-Solid Rocket Company, Sacramento, CA (Technical Library), via AFPRO
- 1 Aerospace Corporation, Los Angeles, CA (Technical Library)
- 1 Allegany Ballistics Laboratory, Cumberland, MD (Technical Library)
- 1 Applied Physics Laboratory, JHU, Laurel, MD
- 1 Atlantic Research Corporation, Alexandria, VA

- 3 Chemical Propulsion Information Agency, Applied Physics Laboratory,
Silver Spring, MD
P. L. Nichols (1)
- 2 Colorado State University, Department of Atmospheric Science
(Arlin J. Krueger)
- 1 Hercules, Incorporated, Bacchus, UT
- 1 IIT Research Institute, Chicago, IL (Document Librarian for
Department M)
- 1 Jet Propulsion Laboratory, CIT, Pasadena, CA (Technical Library)
- 1 Lockheed Propulsion Company, Redlands, CA
- 1 McDonnell Douglas Corporation, Santa Monica, CA
- 1 Midwest Research Institute, Kansas City, MO (Technical Library)
- 1 New Mexico State University, Las Cruces, NM (Physical Sciences
Laboratory, B. G. Gammill)
- 1 Princeton University, Forrestal Campus Library, Princeton, NJ
- 1 Rocketdyne, Canoga Park, CA (Technical Library)
- 1 Rocketdyne, McGregor, TX
- 1 SenTran Company, Santa Barbara, CA (Peter G. Simeth)
- 1 Stanford Research Institute, Menlo Park, CA (Propulsion Sciences
Division)
Technical Library
- 1 Thiokol Chemical Corporation, Bristol, PA (Technical Library)
- 1 Thiokol Chemical Corporation, Elkton, MD (Technical Library)
- 1 Thiokol Chemical Corporation, Huntsville Division, Huntsville,
AL (Technical Library)
- 1 Thiokol Chemical Corporation, Wasatch Division, Brigham City, UT
- 1 United Technologies, Chemical Systems Division, Sunnyvale, CA
(Technical library)
- 1 University of California Lawrence Radiation Laboratory, Livermore,
CA (Technical Information Division)